A Finite Element-Based Phase Field Model

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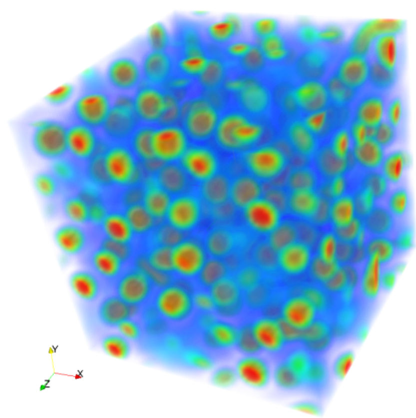
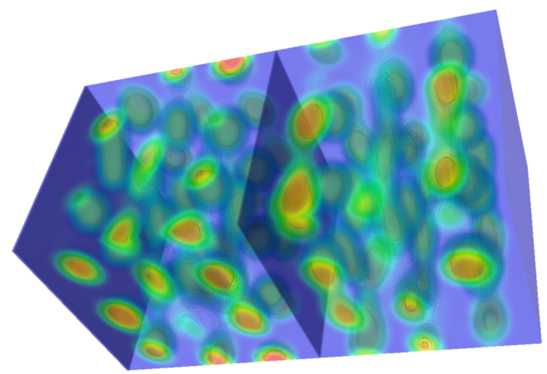
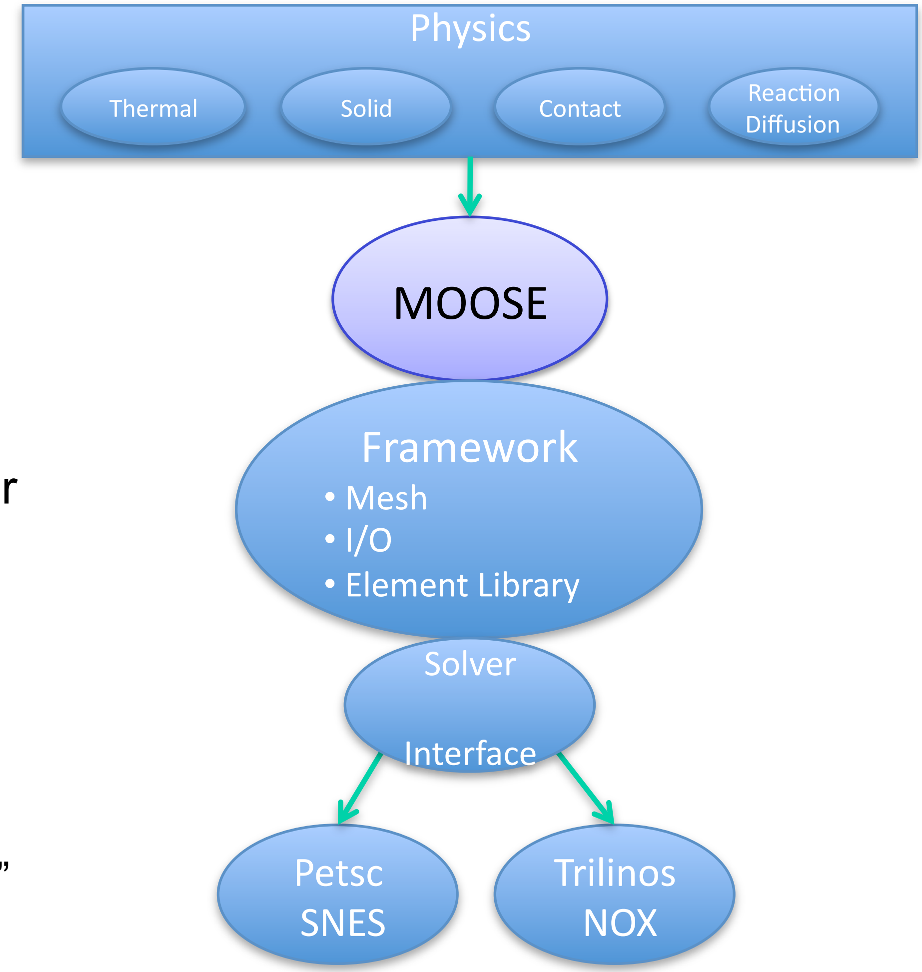




Multiscale Object Oriented Simulation Enviornment (MOOSE)

- Plug-and-play modules
  - Simplified coupling
- MOOSE provides a set of interfaces
- Framework provides core set of common services
  - libMesh: http://libmesh.sf.net
- Solver Interface abstracts specific solver implementations.
  - Common interface to linear and non-linear solvers
  - More flexible
- Utilize state-of-the-art linear and non-linear solvers
  - Robust solvers are key for “ease of use”



Finite Element Solution of Phase Field Equations

- Strong Form

$$
\begin{aligned}
\mathbf{R}_{c_i} &= \frac{\partial c_i}{\partial t} - \nabla \cdot \left(M_{ij} \nabla \left(\frac{\partial g_0}{\partial c_i} - \kappa \nabla^2 c_i + \frac{\partial E_{el}}{\partial c_i} \right) \right) = \mathbf{0} \\
\mathbf{R}_{\eta_i} &= \frac{\partial \eta_i}{\partial t} - L_i \left(\frac{\partial f_0}{\partial \eta_i} - \kappa \nabla^2 \eta_i + \frac{\partial E_{el}}{\partial \eta_i} \right) = \mathbf{0} \\
\mathbf{R}_{\mathbf{u}} &= \nabla \cdot (\boldsymbol{\mathcal{C}}\, \nabla \mathbf{u}) - \nabla \cdot (\boldsymbol{\mathcal{C}} \boldsymbol{\epsilon}^*) = \mathbf{0} \\
\mathbf{R}_T &= \nabla \cdot (k \nabla T) = \mathbf{0}
\end{aligned}
$$

- Weak Form

$$
\begin{aligned}
\mathbf{R}_{c_i} &= \left(\frac{\partial c_i}{\partial t}, \phi_i \right) + \left(M_{ij} \nabla \frac{\partial g_0}{\partial c_i}, \nabla \phi_i \right) + \left(\kappa \nabla^2 c_i, \nabla \cdot (M_{ij} \nabla \phi_i) \right) + \left(M_{ij} \nabla \frac{\partial E_{el}}{\partial c_i}, \nabla \phi_i \right) = \mathbf{0} \\
\mathbf{R}_{\eta_i} &= \left(\frac{\partial \eta_i}{\partial t}, \phi_i \right) + L_i \left(\frac{\partial f_0}{\partial \eta_i}, \phi_i \right) + \kappa \left(\nabla \eta_i, \nabla \phi_i \right) + \left(\frac{\partial E_{el}}{\partial \eta_i}, \phi_i \right) = \mathbf{0} \\
\mathbf{R}_{\mathbf{u}} &= (\boldsymbol{\mathcal{C}}\, \nabla \mathbf{u}, \nabla \phi_i) - (\nabla \cdot \boldsymbol{\mathcal{C}} \boldsymbol{\epsilon}^*, \phi_i) = \mathbf{0} \\
\mathbf{R}_T &= (k \nabla T, \nabla \phi_i) = \mathbf{0}
\end{aligned}
$$

- FEM discretization

$$c_i(\mathbf{r}) = \sum_{j=1}^{N} c_i^j \phi_j(\mathbf{r})$$

Discretized using 3rd order Hermite element

2D: 20 DOF

3D:36 DOF

$$\eta_i(\mathbf{r}) = \sum_{j=1}^{N} \eta_i^j \phi_j(\mathbf{r})$$

Discretized using 1st order Lagrange elements

2D: 8 DOF

3D: 12 DOF

$$\mathbf{u}(\mathbf{r}) = \sum_{j=1}^{N} \mathbf{u}^j \phi_j(\mathbf{r})$$

Discretized using 1st order Lagrange elements

2D: 8 DOF

3D: 12 DOF

$$T(\mathbf{r}) = \sum_{j=1}^{N} T^j \phi_j(\mathbf{r})$$

Discretized using 1st order Lagrange elements

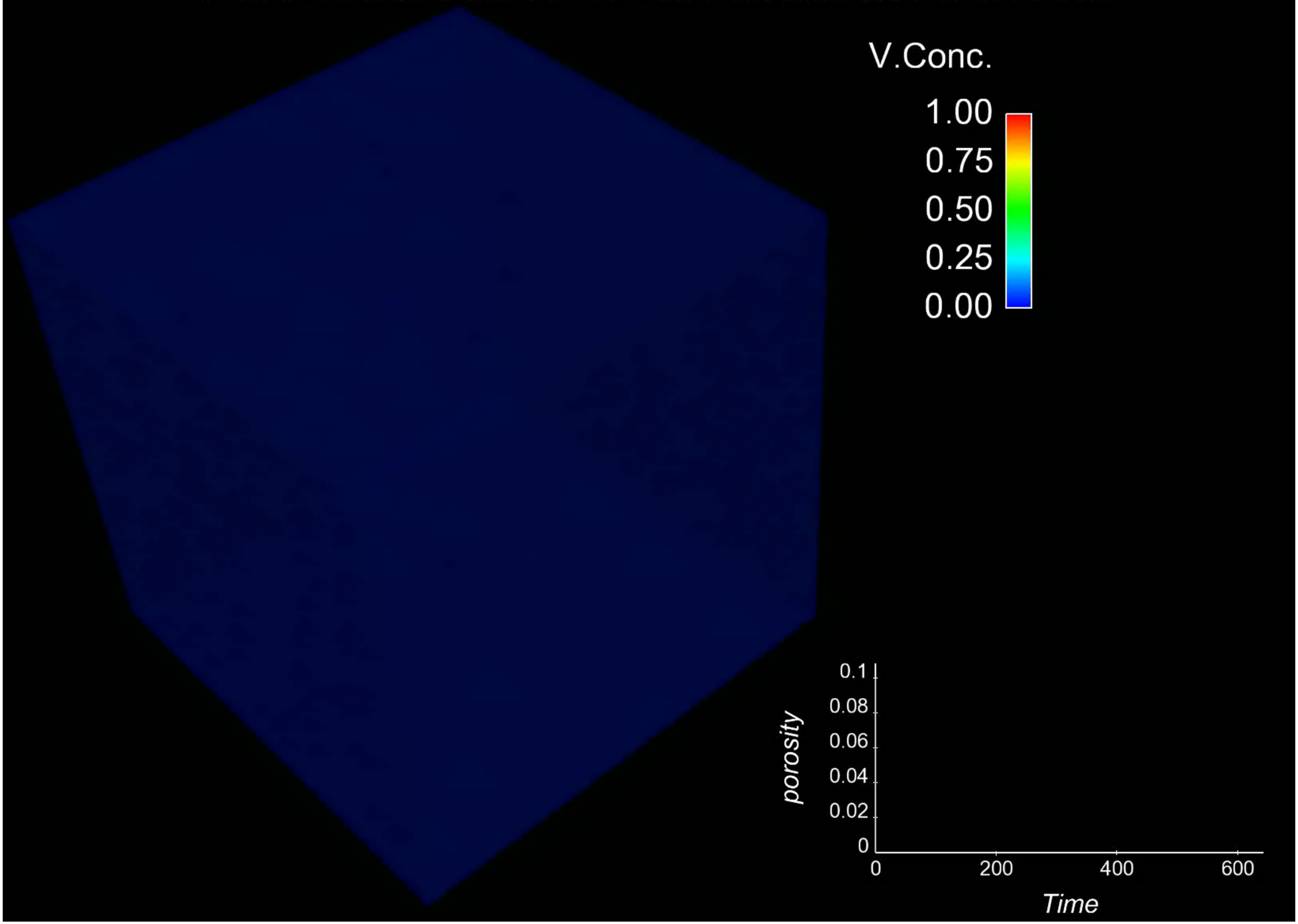
2D: 8 DOF

3D: 12 DOF

MARMOT Summary

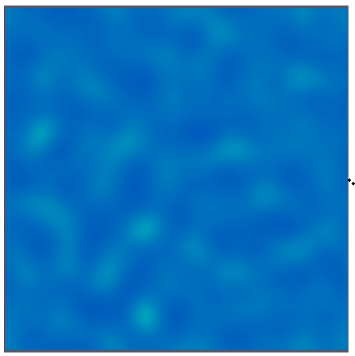
- Implicit solution of the phase field equations using preconditioned JFNK
  - Void nucleation and growth in an irradiated single component metal
  - Grain growth and GB sink effects
- Fully-coupled multiphyiscs – Heat conduction and linear elastic solid mechanics
- Calculation of bulk properties such as effective thermal conductivity and porosity
- Mesh adaptivity
- Time step adaptivity

Void Nucleation in an Irradiated Metal

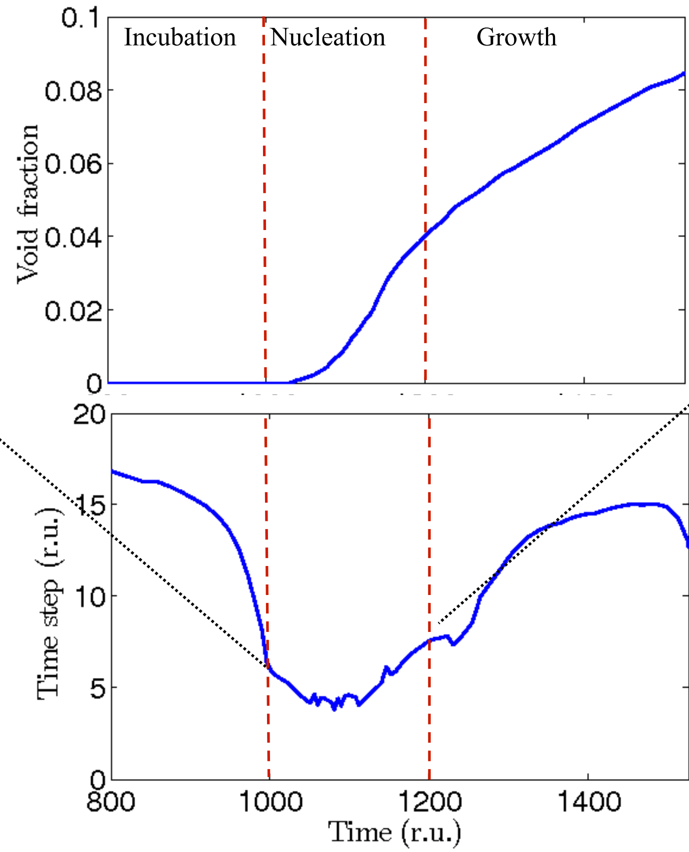


Adaptive Time Step

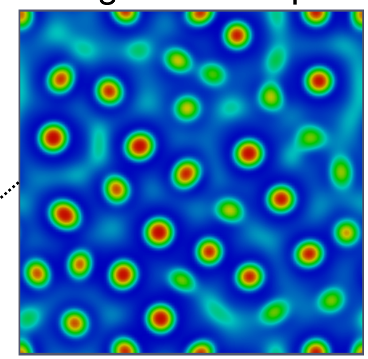
- Solution time step adapts to the current phenomena



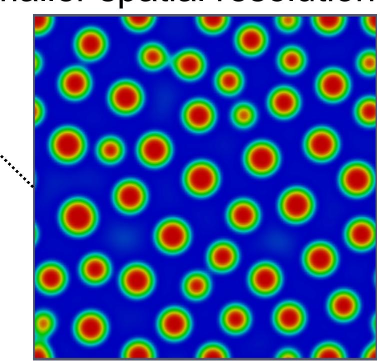
Void nucleation requires small spatial resolution



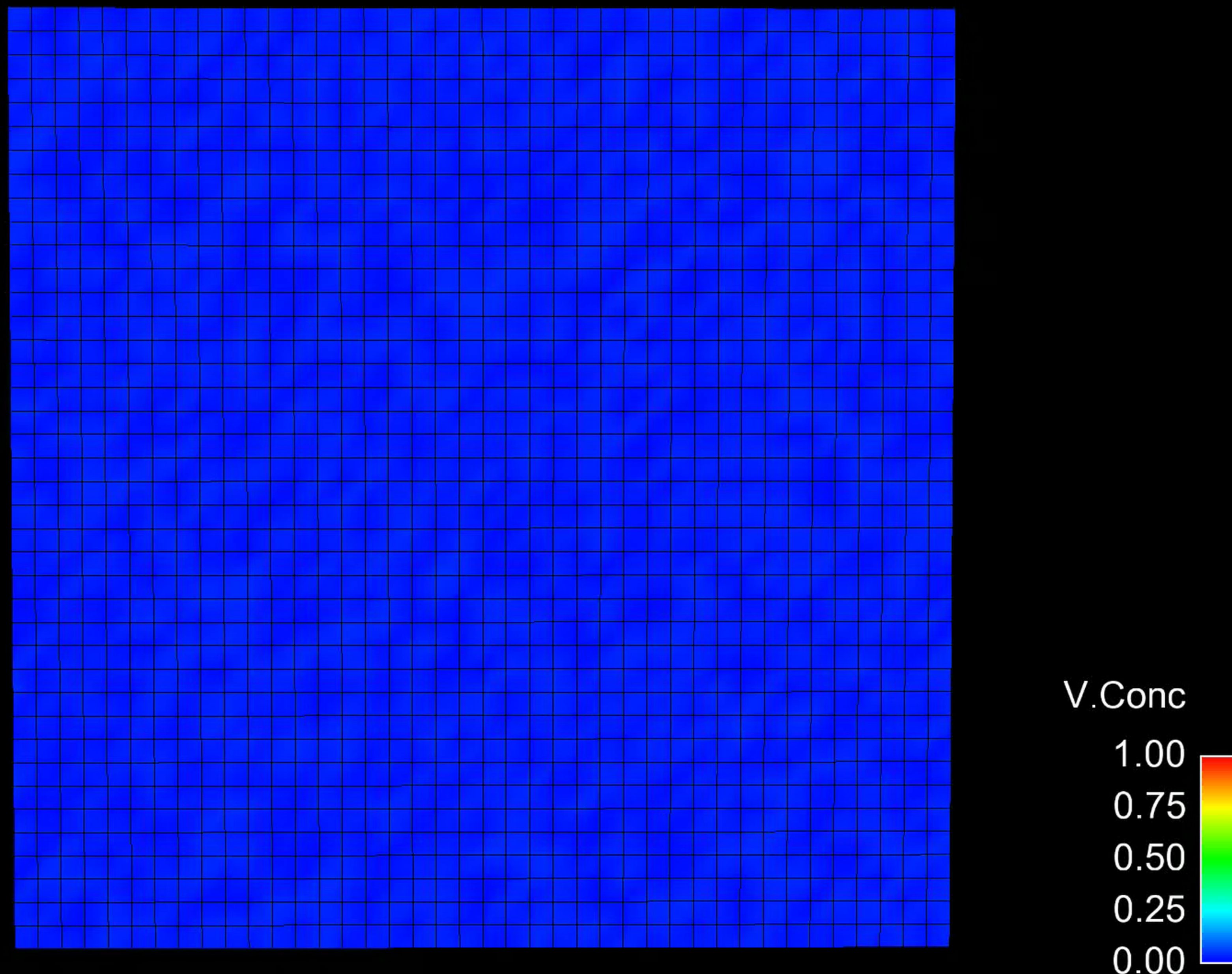
Void growth can be resolved with a larger time step



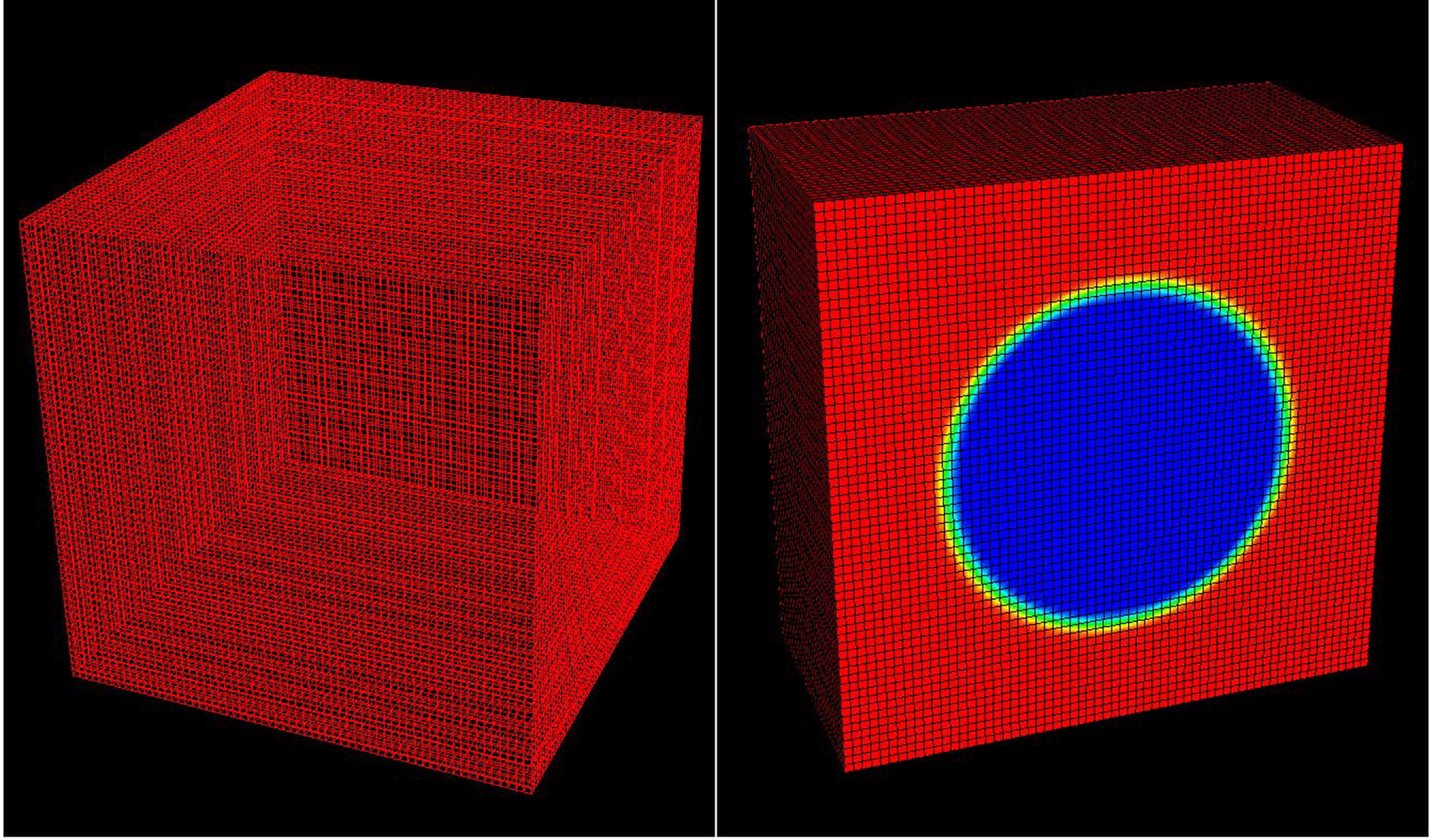
Void coalescence needs smaller spatial resolution

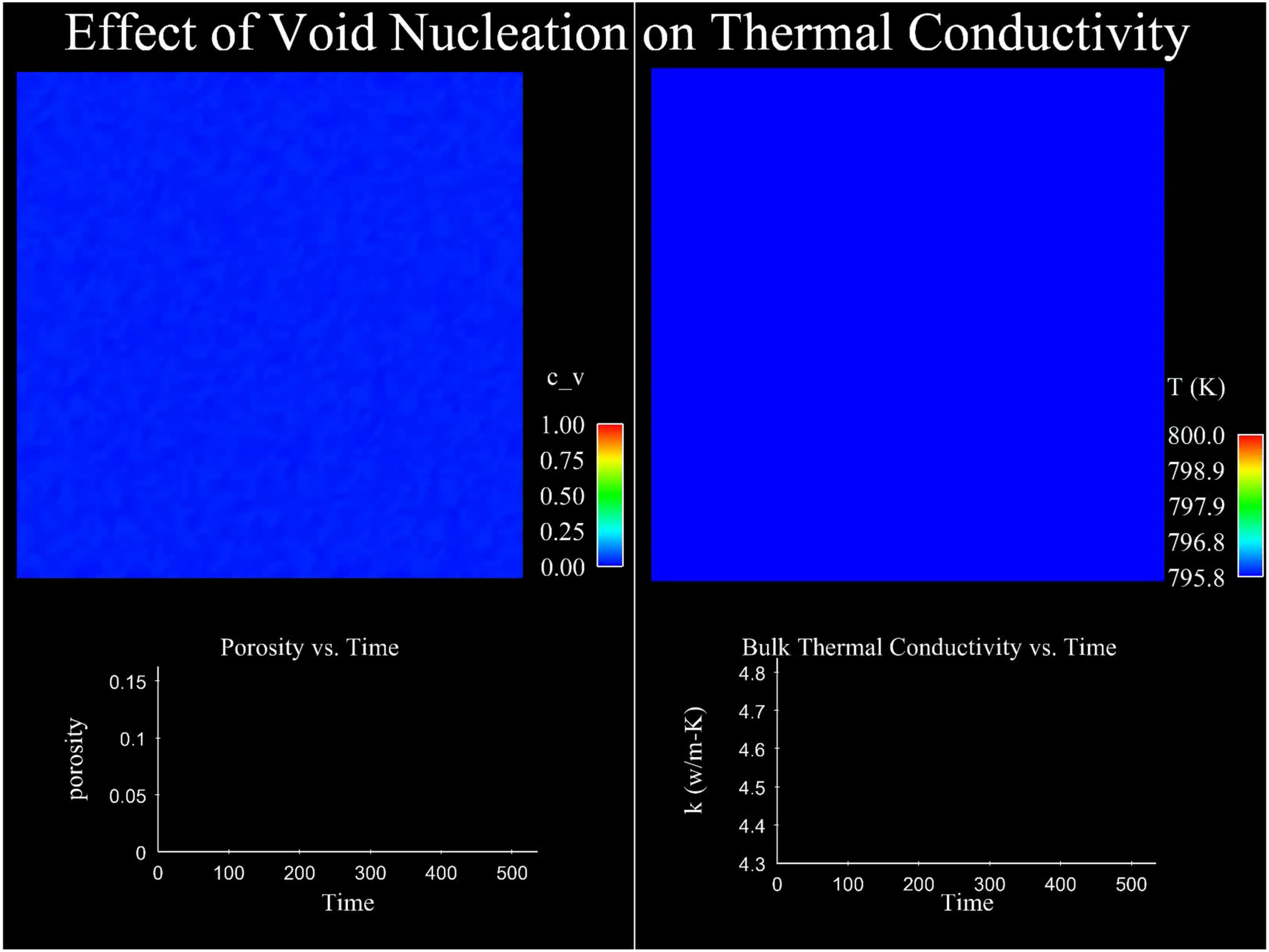


Void Nucleation with Mesh Adaptivity



Shrinking Spherical Grain with Mesh Adaptivity




Effect of Void Nucleation on Thermal Conductivity
c_v
1.00
0.75
0.50
0.25
0.00
T (K)
800.0
798.9
797.9
796.8
795.8
Porosity vs. Time
porosity
0.15
0.1
0.05
0
0
100
200
300
400
500
Time
Bulk Thermal Conductivity vs. Time
k (w/m-K)
4.8
4.7
4.6
4.5
4.4
4.3
0
100
200
300
400
500
Time

Numerical Summary

- Convergence is excellent
- Scalability seems good (we still need to do a full scalability analysis)
- Third-order Hermite elements are expensive. We are currently trying to substitute in an additional variable for the Laplacian interfacial term to allow for linear Lagrange elements.
- Sharp transition in the free energy functional due to the log terms eventually causes problems in the numerical solution

$$f^{solid} = E_v^f c_v + E_i^f c_i + E_g^f c_g + k_B T\left[c_v \ln(c_v) + c_i \ln(c_i) + c_g \ln(c_g) + (1 - c_v - c_i - c_g)\ln(1 - c_v - c_i - c_g)\right]$$